Monte Carlo Sampling Methods Homework 6

Zihan (Steven) Zhang

December 17, 2022

1 Exercise 71

In this question, we need to use a Metropolized version of the overdamped stochastic Newton scheme to sample from the Rosenbrok density:

$$\pi(x) \propto \exp\left(-\frac{100(x_2 - x_1^2)^2 + (1 - x_1)^2}{20}\right).$$
 (1)

When S is a 2×2 matrix with $trace(S) \neq 0$, the matrix:

$$R = \frac{S + \sqrt{\det(S)}I}{\sqrt{\operatorname{trace}(S) + 2\sqrt{\det(S)}}}.$$
 (2)

is a square root of S. The inverse Hessian, $S = (-D^2 \log(\pi(x)))^{-1}$ will not be positive definite for all x. When it is not, we need to replace the inverse Hessian with the square of the matrix obtained by taking absolute values before each square root in the formula for R. Since we are Metropolizing, we could omit the divergence of the S term in the overdamped proposal step without introducing additional bias, but it may increase the rejection rate. In the lecture note, the stochastic Newton iteration is introduced as:

$$X_h^{(k+1)} = X_h^{(k)} - hH^{-1}\left(X_h^{(k)}\right)\nabla^{\mathrm{T}}V\left(X_h^{(k)}\right) + h\operatorname{div}H^{-1}\left(X_h^{(k)}\right) + \sqrt{2hH^{-1}\left(X_h^{(k)}\right)}\xi^{(k+1)} \tag{3}$$

Also, we compare the performance of this preconditioned scheme to the Metropolized overdamped scheme with S=I. Figure 1 shows the change in the acceptance ratio of these two methods under different time step sizes. Figure 2 and 3 show the respective histogram graph.

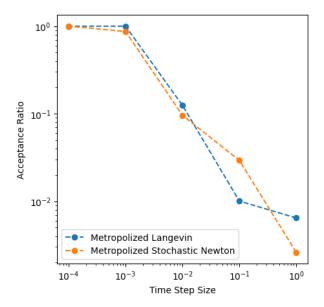


Figure 1: Comparison of Metropolized Langevin and Metropolized Stochastic Newton with under different time step size.

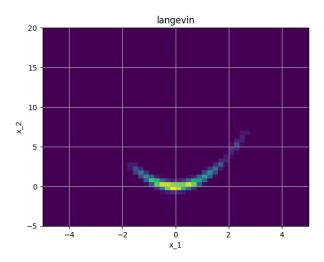


Figure 2: Histogram of Langevin sampling scheme by x_1 and x_2 .

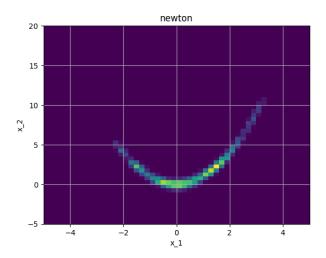


Figure 3: Histogram of Stochastic Newton iteration by x_1 and x_2 .

2 Exercise 75

Here we would use the Affine Invariant Ensemble Scheme (AIES) to sample from the Rosenbrock density defined in the previous. In Figure 4 and Figure 5, we change α and L and observe the change in acceptance rate. In Figure 6, we also plot the graph by x_1 and x_2 for AIES and compare it with section 1. Given the same computational power, in the Rosenbrock problem, the efficiency of preconditioned overdamped Langevin is better than the affine-invariant ensemble sampler, where both are much better than the vanilla overdamped Langevin scheme. Still, this problem is not well-conditioned since the Rosenbrock function cannot be affinely transformed into a nice-shaped function. Also, the narrow nonlinear shape of the density makes the acceptance rate in AIES very low.

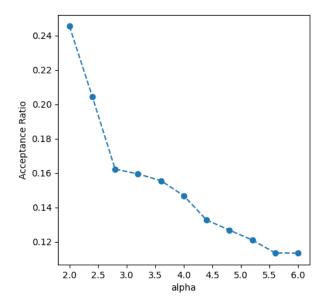


Figure 4: Change of acceptance rate in AIES under different α .

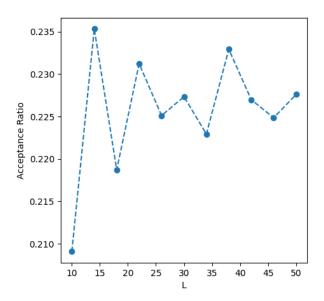


Figure 5: Change of acceptance rate in AIES under different L.

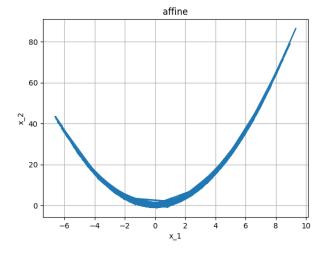


Figure 6: Trajectory of AIES by x_1 and x_2 .